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Simulating Intense Ion Beams for Inertial Fusion Energy

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Science area description

The Heavy Ion Fusion (HIF) program's goal is the development of the body of knowledge needed for Inertial Fusion Energy (IFE) to realize its promise. The intense ion beams that will drive HIF targets are *nonneutral plasmas* and exhibit collective, nonlinear dynamics which must be understood using the kinetic models of plasma physics. This beam physics is both rich and subtle: a wide range in spatial and temporal scales is involved (see figure 1), and effects associated with both instabilities and non-ideal processes must be understood. Ion beams have a "long memory," and initialization of a beam at mid-system with an idealized particle distribution introduces uncertainties; thus, it will be crucial to develop, and to extensively use, an integrated and detailed "source-to-target" HIF beam simulation capability. We begin with an overview of major issues.

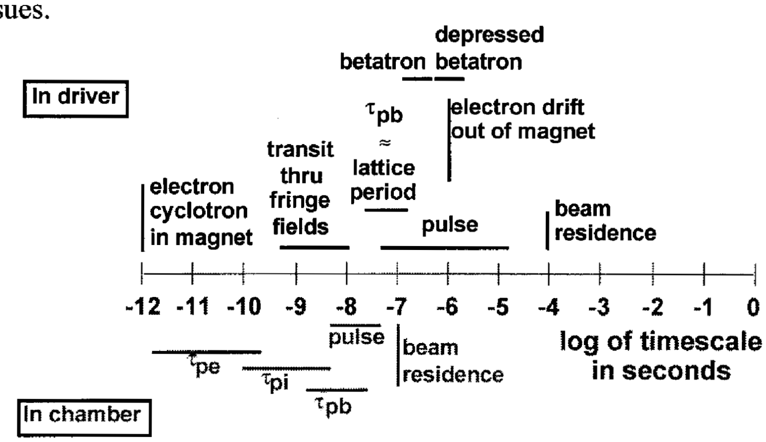

Figure 1. Timescales in driver and fusion chamber. Spatial scale lengths range from electron gyroradii in magnets ~ 0.01 mm, to beam Debye length ~ 1 mm, to beam radius ~ 1 cm, to machine length ~ km's.

Long-term evolution of space-charge-dominated beams: In the driver, the array of beams is accelerated by inductive electric fields, and is confined by applied "focusing" fields. The beams dynamics are "space charge dominated," that is, governed by a balance between the applied fields and space charge forces. This contrasts with the more usual situation in high-energy accelerators, where thermal pressure typically dominates over space charge forces. The beam dynamics is collisionless and Liouvillean, that is, the phase space density remains constant along particle orbits. As a result, "emittance growth" (dilution of the phase space) takes place through complicated distortions driven by collective processes, imperfect applied fields, image fields from nearby conductors and inter-beam forces. Such dilution must be kept minimal, because of the necessity to focus the beams ultimately onto a small (few mm) focal spot on the fusion target. Simulations must capture the effects of small influences which act over long distances. In addition, collective beam modes, and interactions with the external environment which can drive resistive-wall instabilities, must be understood and minimized. Other challenges include the need to accurately simulate time-dependent space-charge-limited emission from curved surfaces, a singular problem. This area is computationally challenging because of the need for an efficient but detailed description of the applied fields, and the needs for good statistics and mesh resolution: 10^7-10^8 particles, ~10^5 steps, more than 100 cells in each transverse direction, and thousands of cells in the longitudinal direction, for a simulation with a co-moving mesh that "treadmills" with the beam.

Beam halo generation: In modern particle accelerators, the confining fields are dominated by an "alternating-gradient" transverse quadrupole moment from a sequence of electric or magnetic lenses. Thus, the confining fields are non-steady in the beam frame, complicating analysis; no exact nonsingular equilibria are known, and it may be that none exist. Oscillations of the beam "core" can parametrically pump particles into an outlying, or "halo," population. For focusability and also to avoid the adverse effects of ions impinging on walls, beam halo must be kept minimal. Here, PIC methods have been used, but emerging continuum-Vlasov and nonlinear-perturbative methods may offer advantages.

Multispecies effects in driver: collective beam interactions with "stray" electrons in the accelerator and transport lines, including electron generation and trapping within the beam, must be understood quantitatively. This area is computationally challenging because of the ratio between the fast time scale for electron motion and the slow time scale for electron build-up within the beam; the need to efficiently gather/scatter and communicate multi-species information for ionization and surface-physics processes; and the needs for efficient dynamic load balancing and perhaps an adaptive mesh. Electron scales in the driver will not be resolved in full end-to-end simulations in the near future, so coupled disparate-timescale simulations capturing electron dynamics and/or "subscale" modeling will be employed.

Beam interactions with fusion chamber environment: 3-D simulations of the propagation of the cluster of beams through the final focusing optics, and onward through the fusion chamber's environment of gas and plasma, are required in order to provide a realistically complete model of the target illumination. The beam and background plasma dynamics include: multibeam effects; return current formation and dynamics (streaming instabilities); imperfect neutralization; beam stripping; emittance growth; and photo-ionization of the beam ions and background gas. Of these effects, many of the greatest uncertainties and computational challenges are associated with multiple-beam interactions near the target, and these will be one important focus of research efforts. Another important focus of research efforts in the fusion chamber will be on collective instabilities, such as resistive hose, filamentation and two-stream modes.

In the chamber as in the driver, it is appropriate to employ multiple methods, and we will use PIC, hybrid PIC-fluid, and nonlinear perturbative ("delta-f") methods. The chamber calculations must allow exploration of various propagation modes, e.g. "neutralized-ballistic," "assisted-pinch," etc. The challenges include the need for complex physics models, "outgoing-wave boundary conditions," an implicit hybrid model for the dense-plasma scenarios, and of order 10^7-10^8 simulation particles. It will also be valuable to employ multiple models, so as to compare, *e.g.*, implicit electromagnetic (EM) methods (which can stably under-resolve fast time scales not essential to the physics) with explicit EM methods and with magneto-inductive ("Darwin") methods that eliminate light waves from the description.

Key computational tools

The HIF program has developed tools to explore these physics areas, primarily (but not exclusively) using particle-in-cell (PIC) methods. Plans involve adaptation of exiting codes to run optimally on computers that use a hybrid of shared and distributed memory, tight coupling between those tools, production of new and improved numerical algorithms, e.g., averaging techniques that allow larger time-steps, and development of improved physics models. Some of this work already relies heavily on modern scripting techniques for code steering, and advanced data visualization is playing an increasing role. In all areas, benchmarking with theory, with experiments, and among codes will continue to be essential.

The codes to be improved, coupled, and employed are listed in Table 1. All are well-positioned to move quickly to the new hardware platform. WARP and LSP are fairly large and complex codes offering many options; they are, more accurately, code frameworks. BEST and BPIC are smaller codes that are attractive test-beds for new methods, in addition to being useful tools in their own right. The majority of the required simulations are between one and two orders-of-magnitude beyond current practice; we anticipate typical run times of order a day. Here we characterize the codes by their methods, and by their regimes of applicability.

Follow particles (plasma particle-in-cell method)
- WARP (driver): 3-D (or r,z or x,y) ES, detailed lattice
- LSP (chamber & driver): 3-D or (r,z) implicit (or explicit) EM or ES, hybrid (kinetic/fluid)
- BPIC (chamber): 3-D or (r,z) EM, moving grid, outgoing waves

Follow particles and perturbation to distribution function (δf)
- BEST (chamber & driver): 3-D EM, Darwin, or ES, offers reduced noise

Evolve distribution function (f) on a grid
- WARP-SLV (driver): 2-D (x,y,p_x,p_y) ES Semi-Lagrangian Vlasov solver

Evolve moments of distribution function
- WARP-CIRCE & WARP-HERMES (driver): transverse moments, longitudinal Lagrangian fluid

Table 1. Classes of codes for HIF beams, codes in use or being developed, and domains of applicability

WARP offers 3D and transverse-slice 2-1/2D geometries, and is used extensively throughout the Heavy Ion Fusion program for studies of beams in the accelerator, pulse-compression line, and final focusing system. WARP runs in parallel on NERSC's Cray T3E-900 and IBM SP, using message passing. Good scaling has been obtained using up to 256 processors on problems of intermediate size. The code is written in a coarse-grained object-oriented superset of Fortran, and runs under the control of the Python scripting language. A prototype continuum Vlasov package, SLV, was implemented in the WARP code and is currently running on simple axisymmetric beam physics problems. Moment based models CIRCE and HERMES, useful for rapid scoping and synthesis, are also implemented within the WARP framework.

LSP offers (r,z) and 3D geometries, implicit or explicit EM or ES PIC and fluid models, a multi-block mesh which allows simulation of non-rectangular (*e.g.*, L-shaped) regions, and domain decomposition designed for multilevel memory access. Its implicit hybrid model enables simulation of dense-plasma scenarios. LSP has extensive gas and surface interaction physics models; it already offers secondary emission, kinetic neutrals, ionization, scatter and neutral recycling, and has achieved good scaling using up to 256 processors on problems of intermediate size. LSP is written in C using an object-oriented style.

The BPIC chamber-propagation code offers an explicit 3-D or (r,z) electromagnetic PIC model, and uses a time-evolving mesh and uses novel methods for "advecting away" the field errors associated with the evolving cell boundaries. It is written in Fortran 95.

BEST offers nonlinear-perturbative ("delta-f") simulation in 3D geometry and has been parallelized using a combination of MPI and OpenMP and two-dimensional domain decomposition suitable for a supercomputer equipped with both shared and distributed memory. The code was designed to elucidate mode structures by minimizing discrete-particle noise, employs a new Darwin (magnetoinductive) model algorithm, and, to compensate for the mass ratio (about 250,000) of the heavy ions to the electrons, uses a newly-developed adiabatic pushing and deposition algorithm. Good scaling has been obtained using up to 512 processors. It is written in Fortran 95.

Representative simulations

Existing codes are used for a wide variety of simulations, as illustrated in Figure 2. We do not attempt to describe the relevant physics in any detail, but merely show the range of ongoing activities.

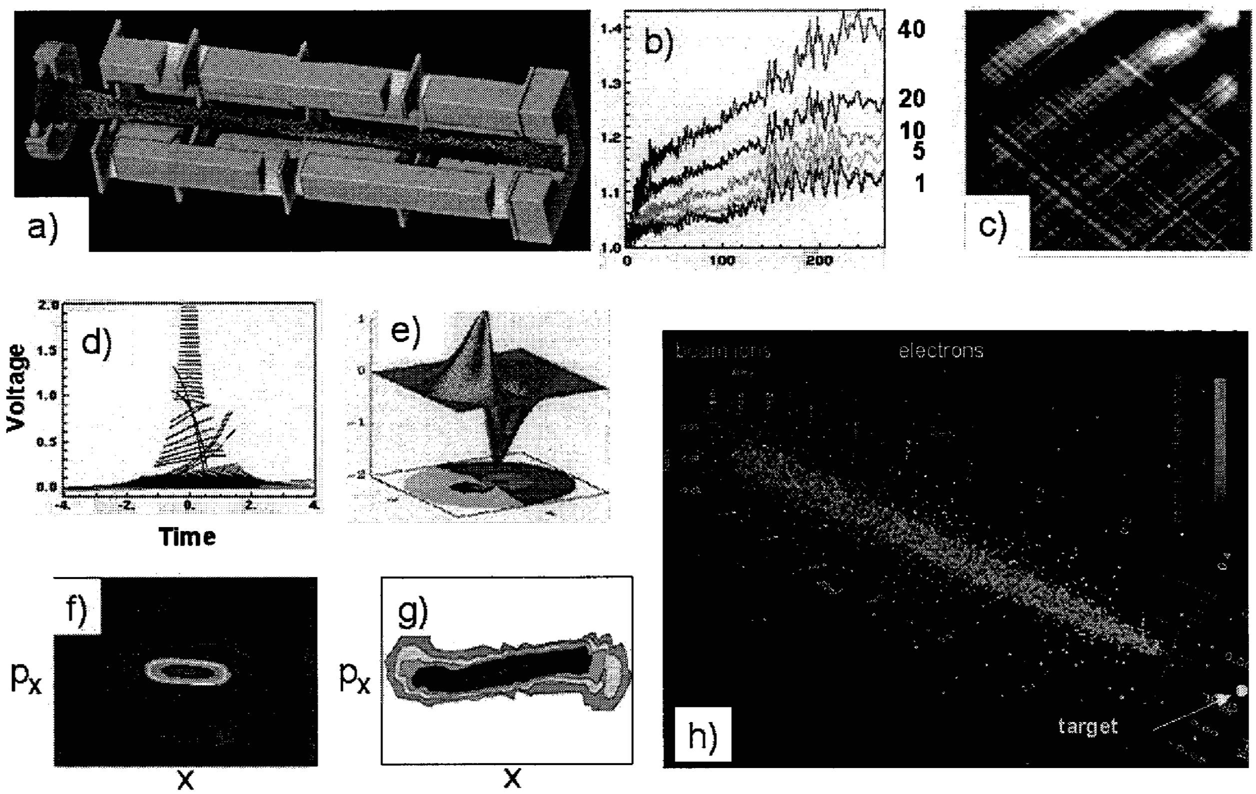

Figure 2. Representative output from HIF beam simulations: (a) WARP3d simulation of space-charge-limited emission off a curved surface, and acceleration in a 3-D structure, including subgrid-scale placement of conductor boundaries (cut-cell method); (b) WARPxy study of beam emittance versus time in an imperfectly-aligned beamline, for five different intervals between applications of steering.; (c) WARP3d study of longitudinal waves on beam, driven unstable by impedance of accelerating structures; (d) accelerating waveforms for a possible future experimental accelerator, for use in WARP3d simulations; (e) BEST simulation of unstable electron-ion two-stream mode in a beamline; (f) semi-Lagrangian Vlasov simulation of beam halo generation due to anharmonic focusing fields, using prototype model in WARP-SLV; (g) distorted beam phase space in final focusing, as simulated using WARPxy; (h) BPIC simulation of beam transit through fusion chamber environment and onto the target.

Approach

A concept for source-to-target simulation is shown in Figure 3. In this scenario, the beam is simulated from the source through the final focusing optic using WARP3d, and the particle and field data are then transferred into LSP (or BPIC) where the simulation is carried through to the fusion target. At that point the particle data is used to generate "ray" information for the ion beam source in the target simulation code. Meanwhile, LSP is used to study electron effects in the driver, especially sources and trapping in the beam;

for this to be accurate, it is necessary to understand beam halo quantitatively, and for this the marker-following capabilities of BEST and/or the Vlasov solver in WARP are employed in coupled side calculations. BEST is also used to study beam instabilities in detail, using parameters transferred from WARP and LSP.

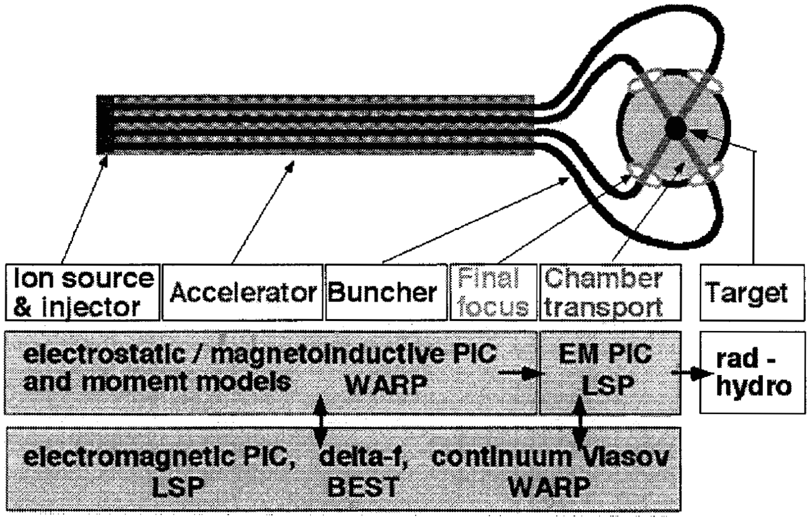

Figure 3. Depiction of source-to-target simulation strategy (see text)

The major developments required include: (i) optimization of codes for efficiency on the new computer architecture; (ii) development of new and improved numerical algorithms (*e.g.*, for larger timesteps and Vlasov solution); and (iii) development of improved physics models (*e.g.*, for multibeam, converging beam, self-magnetic, atomic physics, and module impedance effects) that will be made practical by the terascale capability. The codes will be linked using scripting tools (especially Python) for intercommunication and code steering, "workspace" tools for heterogeneous computations, and self-describing data files (*e.g.*, NetCDF). The "data glut" associated with saving information from the many processors will be addressed by incorporating optimized parallel I/O capabilities. The challenges of visualizing a time-dependent 6D phase space will be addressed through the use of volume and isosurface rendering, coupled with projection and range selection along the non-visualized coordinate directions; animation will also be further developed and employed. The simulations will entail self-consistent field descriptions requiring interprocessor communication, but will employ optimized domain decomposition and dynamic load balancing so as to be scalable on terascale architectures.

Relationships with other scientific disciplines

This research area involves nonlinear dynamics, self-consistent fields, large-scale parallel computations, massive data handling, interactive and script-driven code steering, and visualization of a time-dependent multidimensional phase space. These aspects appear in many emerging applications of terascale computing, and considerable cross fertilization with other areas can be anticipated.

Other accelerator applications are moving toward higher beam intensities, and the knowledge gained via this research into very strong space-charge regimes will be relevant to a wide variety of applications. We anticipate long-term benefits to such efforts as the Spallation Neutron Source, the Very Large Hadron Collider, the Next Linear Collider, the Accelerator for Transmutation of Waste, the Muon Collider, and for application to Boron Neutron Capture Therapy.

HIF researchers are collaborating with the NERSC computational science group in the integration of Adaptive Mesh Refinement (AMR) techniques with the Heavy Ion Fusion PIC simulation code WARP3d. That group initially developed the AMR method for application to combustion and fluid flow studies. We anticipate that the method will be useful in simulation studies of heavy ion beams in several contexts: mesh refinement around the beam in a PIC code; around internal conducting structures to capture subtle but important field details; and around key phase-space structures in a continuum Vlasov calculation in 4D, 5D, and ultimately 6D, where straightforward methods would require a very large mesh.

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